

Resorcinol monoacetate
102-29-4 | DTXSID6045901

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.79

Global applicability domain: Inside

Local applicability domain index: 5.11e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde

Measured: 3.02

Predicted: 2.77

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

Image not found

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

Image not found

2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35

Image not found

Sulfolane

Measured: 7.08

Predicted: 6.91